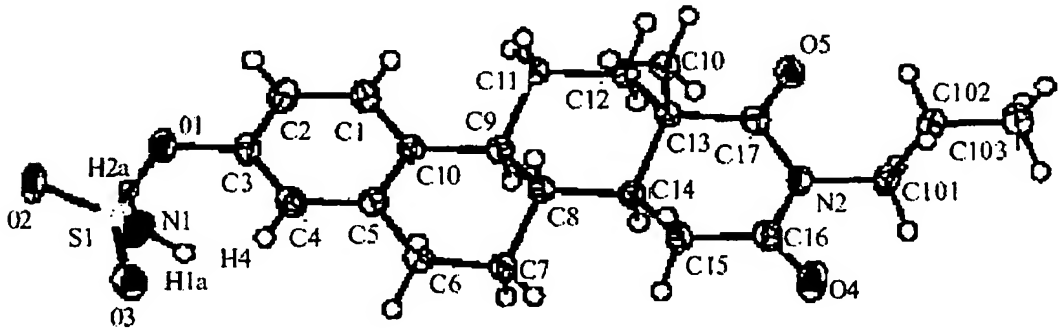
optimum when the alkyl group was an heptyl moiety. Their potency, similar to that of EMATE, clearly underlines the presence of a hydrophobic pocket in the enzyme active site corresponding to the direction of the 17β-substituent.

A weaker inhibition of STS by **41** therefore suggests that the orientation of its side-chain, situated on the N-atom of the D-ring (6-membered), is different enough from that of the 17β-side-chain of **1** or **2** (5-membered D-ring) to induce a decrease of affinity with the active site of the enzyme. It can be proposed that, while there is a hydrophobic pocket in the enzyme active site for 17β-substituents, the topology of the active site around the N-position of a 6-membered ring could be more restrictive to bulky substituents. To corroborate this hypothesis, molecular modelling would be a tool of choice.

In order to elucidate the orientation of the atoms in the D-ring and in the side-chain, as well as gather data for possible future molecular modelling studies, the crystal structure of the highly potent oestrone derivative **39** was determined. A crystal (approx. dimensions 0.20×0.17×0.08 mm), obtained from slow recrystallization in acetone/hexane, was used for data collection.

The ORTEP plot of the asymmetric unit of **41** is shown below along with the labelling scheme used. The sulfamate group, all four rings, and the key features of the modified D-ring are clearly visible. As expected, the D-ring is in a half chair conformation since the imide function implies the position of the atoms C13, C17, N and C1' as well as C15, C16, N and C1' in the same plan.



ORTEP plot of the X-ray crystal structure of **41**. Ellipsoids are shown at the xx% probability level.